

**ECE 495N**

# **Fundamentals of Nanoelectronics**

**Fall 2008**

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**Lecture: 18  
Title: Bandstructures I  
Date: October 10, 2008**

**Video Lectures posted at:  
<https://www.nanohub.org/resources/5346/>**

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# Bandstructures I

## Lecture 18

Oct. 10, 2008

$$E\Phi = \left[ -\frac{\hbar^2}{2m} \nabla^2 + U \right] \Phi$$

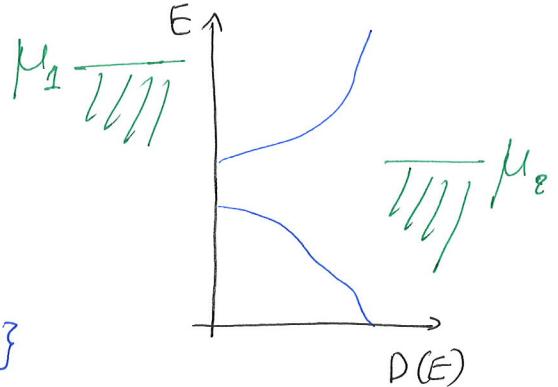
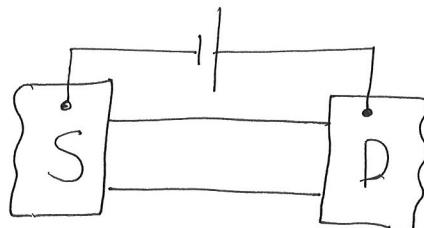
$\equiv H_{\text{op}}$

$$\Phi(\vec{r}) = \sum_m \phi_m \underbrace{u_m(\vec{r})}_{\text{basis functions}}$$

$$E[S]\{\phi\} = [H]\{\phi\} \xrightarrow{S=I} E\{\phi\} = [H]\{\phi\}$$

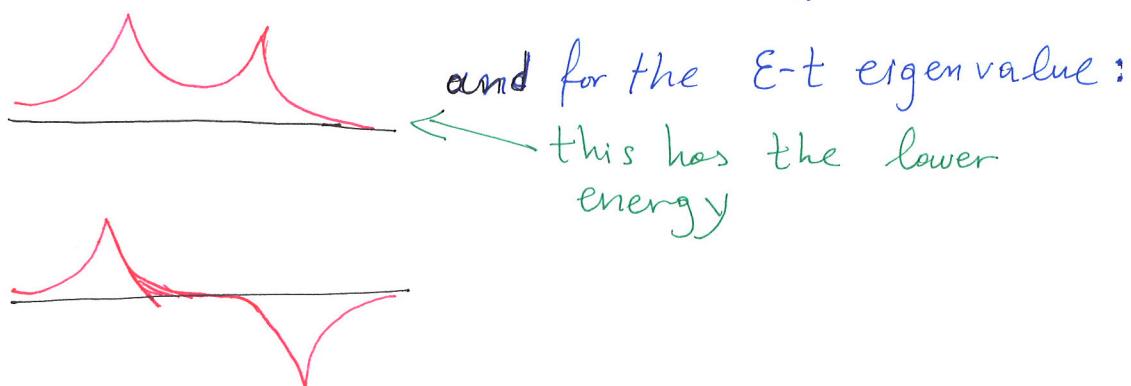
$$H_{mn} = \int d\vec{r} u_m H_{\text{op}} u_n$$

$$S_{mn} = \int d\vec{r} u_m u_n$$



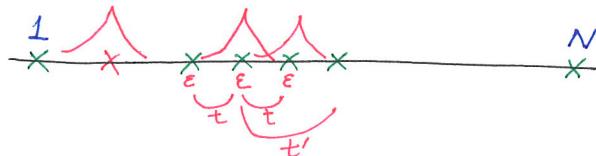
$$\begin{array}{c} \text{H-H} \\ \xrightarrow{\text{generally}} \begin{bmatrix} \epsilon' & t' \\ t' & \epsilon' \end{bmatrix} \xrightarrow{\text{for } H_0} \begin{bmatrix} \epsilon & t \\ t & \epsilon \end{bmatrix} \end{array}$$

with eigenvalues  $\epsilon+t$ ,  $\epsilon-t$  and eigenvectors  $(1), (-1)$ . The solution will be for the  $\epsilon+t$  energy level:



The problem is when we have a solid which has many atoms because the matrix is very huge.

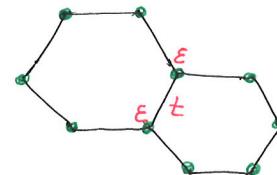
This problem is simplified if we use the property of Periodicity:



$$t' \ll t \Rightarrow \text{nearest neighbor model} \\ \Rightarrow t' = 0$$

$$H = \begin{bmatrix} \varepsilon & t & t' & & & \\ t & \varepsilon & t & t' & & \\ t' & t & \varepsilon & t & t' & \\ & t' & t & \varepsilon & t & t' \\ & & t' & t & \varepsilon & t \\ & & & & \ddots & \ddots \\ & & & & & \varepsilon \end{bmatrix}$$

Other example is the graphine:

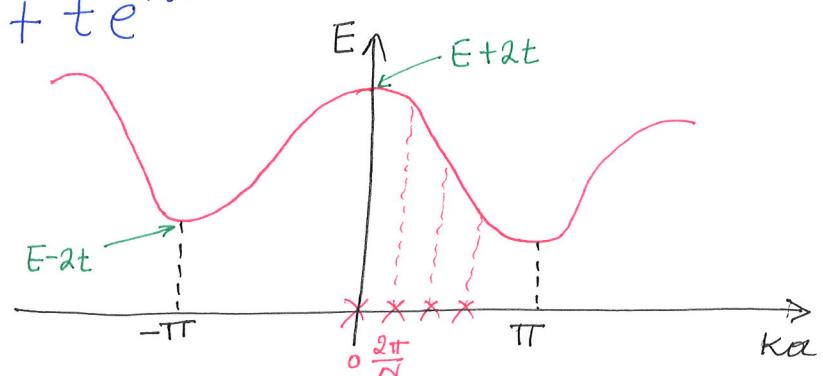


$$E \cdot \begin{Bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_N \end{Bmatrix} = \begin{bmatrix} \varepsilon & t & & & & \\ t & \varepsilon & t & & & \\ & t & \varepsilon & t & & \\ & & t & \varepsilon & t & \\ & & & t & \varepsilon & t \\ & & & & t & \varepsilon \end{bmatrix} \cdot \begin{Bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_N \end{Bmatrix} \xrightarrow{\text{Periodic boundary condition}} \begin{aligned} E\phi_n &= t\phi_{n-1} + \varepsilon\phi_n + t\phi_{n+1} \quad \textcircled{A} \\ &\text{for } n = 1, \dots, N \end{aligned}$$

This solution:  $\phi_n = \phi_0 e^{in(k\alpha)}$  satisfy the equation  $\textcircled{A}$ . If we substitute in  $\textcircled{A}$  we have:

$$E\phi_0 e^{in(k\alpha)} = t\phi_0 e^{i(n-1)k\alpha} + \varepsilon\phi_0 e^{in(k\alpha)} + t\phi_0 e^{i(n+1)k\alpha}$$

$$\xrightarrow[\substack{(\cdot) \\ e^{-ink\alpha}}]{} E = t e^{-ik\alpha} + \varepsilon + t e^{+ik\alpha} \\ = \varepsilon + 2t \cos k\alpha$$



In addition we have boundary condition. For this case we are taking Periodic boundary condition (PBC) which means

$$\phi_N = \phi_1 \Rightarrow \phi_N = \phi_0 e^{i N k a} = \phi_0 \Rightarrow e^{i N k a} = 1$$

$$\Rightarrow N k a = \frac{Q \pi}{N} \text{ (integer)}$$

If I take a <sup>valid</sup> value for  $k a$  and add  $2\pi$  then I'll take the same solution, namely the solutions

$$\phi_n = \phi_0 e^{i n (k a)} \quad \text{and}$$

$$\phi_n = \phi_0 e^{i n (k a + 2\pi)}$$

are the same solutions.